

SIMULATION OF THE STEADY-STATE
AND DYNAMIC BEHAVIOUR OF GENERAL
MULTIPLE EFFECT EVAPORATION PLANTS

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SIMULATION OF THE STEADY-STATE AND DYNAMIC BEHAVIOUR
OF GENERAL MULTIPLE EFFECT EVAPORATION PLANTS

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The thesis consists of this summary and of the following papers:

- I. Bolmstedt, U. and Gudmundson, C.
Improved Methods for Design and Evaluation Calculations
of Multiple Effect Evaporation Plants
Svensk Papperstidning 77(1), 27 (1974)
- II. Bolmstedt, U.
Computer-Aided Simulation of the Dynamic Behaviour
of Multiple Effect Evaporation Plants
To be published

In the following, these papers will be referred to as Part I and Part II, respectively.

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INTRODUCTION

In the field of chemical processing, multiple effect evaporators are often an important part of the process equipment. Typical, well-established applications are those found in the kraft pulp and sugar industries. Furthermore, multiple effect evaporators are commonly used in the food industry, for the concentration of, for instance, tomato juice and skim milk. Another important application is the evaporation of sea-water in the production of fresh water.

In practice, all these different applications require different types of evaporators and moreover, different liquid feed arrangements are used. However, although the various plant arrangements are well established in principle, a large number of modifications can be made within the basic arrangements to obtain better operating conditions. With the present rising energy costs, there is also great interest in modifying the plants for higher efficiency and thereby better plant economy. Minor plant modifications may be based on previously gained experience, but with radically changed plant arrangements there is great uncertainty in using data from plants in conventional operation. Hence it is necessary to perform a number of accurate design calculations in order to determine the usefulness and efficiency of various new arrangements. Accurate calculations are, however, generally very extensive, and furthermore, they are of an iterative nature. Moreover, the extent of the calculations increases rapidly with the complexity of the plant. Considering this, manual calculation methods are hardly applicable.

Instead, a computer seems to be the proper instrument for the treatment of this type of calculations. With a flexible computer program, a large number of different plant arrangements can be accurately calculated with a minimum of effort, and the results can be used as a basis for the determination of a proper plant design. Part I of the present thesis is concerned with the evaluation and application of the computer program INDUNS, designed to calculate multiple effect evaporation plants of arbitrary complexity. The program may be used for design as well as for evaluation calculations of any plant, regardless of the type of solution being evaporated, and regardless of the vapour and liquid schemes being used.

However, only the steady-state characteristics of multiple effect evaporators can be examined with the aid of INDUNS. Since real plants never operate under perfect steady-state conditions, it is clear that the determination of dynamic characteristics can be very useful in the design work. This information can be obtained from dynamic simulations, already at the design stage. Hence the effects of changed operating conditions, for instance disturbances in the feed flow rate or in the feed concentration, are easily studied. Furthermore, dynamic simulations may be used to facilitate the determination of proper controller settings of liquid level controllers, *etc.* Part II of the present thesis is concerned with the evaluation and suggested application of the computer program DYNEFF, designed to be used primarily for the simulation of open-loop responses of general multiple effect evaporation plants. However, it should also be possible to use DYNEFF for identification purposes, *i.e.* for the determination of low-order models, applicable to computer control of evaporation plants.

STEADY-STATE SIMULATION

Generally, steady-state calculations of multiple effect evaporation plants involve the solution of a system of heat and mass balances. This applies to evaluation as well as design calculations, but normally the latter are much more extensive.

Due to the complicated relationships among many of the variables involved, a great number of data must be estimated, more or less accurately, in the initial stage of the calculations. Hence some iterative solution technique must be used. In order to facilitate the solution procedure some authors, *e.g.* Hassett¹ (1957), Freund² (1963), Militzer³ (1965), and Wiklund⁴ (1968), have developed methods applicable to multiple effect evaporator calculations. Others, *e.g.* Wise⁵ (1960) and Oden⁶ (1967), propose graphical methods. However, the methods are in most cases of the "short-cut" type, and are therefore not suitable for accurate calculations. Besides, they are often very restricted with respect to feed arrangements, *etc.*

Computer programs

Evidently, there are many difficulties involved in the use of a manual calculation method. Due to the iterative nature of the calculations, a computer seems to be a suitable instrument for the solution procedure. The first paper on a computer program for this type of problems was presented by Marek⁷ (1962). Naturally, the program was very simple due to the limitations of the computers available in 1962, and could handle only very restricted design calculations. Since 1962, some ten computer programs designed for multiple effect evaporation plant calculations have been reported. However, when only "general" programs are considered, *i.e.* programs not restricted to a certain type of calculations, to a certain flow scheme, or to certain physical data, only a few programs can be found in the literature. The first program of this kind was reported by Jernqvist *et al.*⁸ (1966). The basic ideas of the program, called EVAPOCHALM, were the description of the plant flow sheet with the aid of a "unit cell" and a "connection matrix". Another program, presented by von Schalien *et al.*⁹ (1970), was designed using some ideas of EVAPOCHALM.

In an earlier report¹⁰ (Bolmstedt, 1971), a comprehensive literature survey on both digital and analog computer programs for multiple effect evaporator calculations is given. In another report¹¹ (Bolmstedt, 1972), some of these

programs are discussed in detail.

The computer program INDUNS

An examination of the published programs indicated that there was still much to do in this field. Therefore, a research project was started to construct a program more "up-to-date" than those mentioned above. From the analysis of the programs it was determined that certain ideas presented by Jernqvist *et al.*⁸ (1966) should be used in the design work. Hence the principles of a modular composition of evaporation plant flow sheets with the aid of a unit cell, and the description of the flow sheet with the aid of a connection matrix, were considered suitable for further development. Some of the demands upon the new program, called INDUNS, were for instance maximum flexibility, minimum computer running times, a simple data input procedure, and assured convergence even for very complicated calculation cases.

The unit cell of INDUNS, shown in figure 1, was designed to provide maximum flexibility, as well as maximum simplicity of the flow sheet data input procedure. The number of unit cells is, in principle, unlimited. The following equipment is included in one unit cell:

- evaporator vessel
- thermo-compressor
- condensate and solution flash tanks; maximum number: 5
- condensate level controller
- heat exchangers; maximum number: 9
- liquid mixing/division vessels; maximum number: 5
- vapour mixing/division vessels; maximum number: 5

In figure 1 some streams are alternatively marked with dashed lines and empty arrows. This means that they diverge from the so-called "standard-connections" within the unit cell. The purpose of the standard connections is to facilitate the establishment of the connection matrix in most cases. Thus all equipment within one unit cell is normally connected according to the solid lines. Consequently, the heat exchangers are heated by the same steam as the evaporator vessel, all the condensate streams are mixed, and the flash tank vapour is mixed with the steam to the evaporator vessel, unless contradictory data are given by the user.

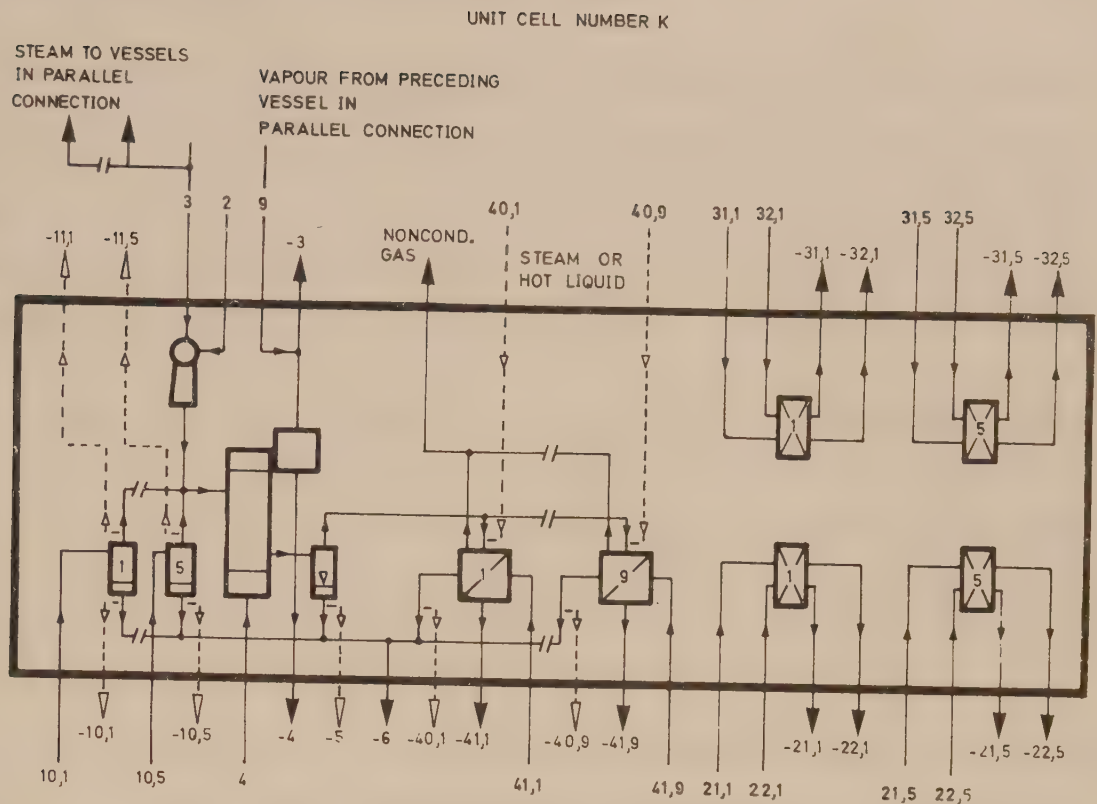


Figure 1. The unit cell

The streams designed to be used only for parallel connections on the vapour side are shown in figure 1. These streams are denoted "steam to vessels in parallel connection" and "vapour from preceding vessel in parallel connection". With the aid of these streams only, the most "tricky" combinations of parallel vapour lines and parallel vessels can be easily set up and described with the aid of the connection matrix.

In INDUNS, the internal matrix row numbers are not used for the identification of variables. Instead, a system of mnemonic symbols is used. This facilitates the data input procedure and makes the output of data very clear. Each symbol consists of six alpha-numerical characters. For the liquid and vapour streams, all data are presented in uniform "data blocks" in the data output matrix. Mnemonic symbols are also assigned to some supplementary data belonging to the liquid mixing/division vessels, the vapour mixing/division vessels, and the heat exchangers. Furthermore, symbols are assigned to some miscellaneous data, not belonging to any of the liquid or

vapour streams. Such data are for instance boiling point elevation, boiling temperature of evaporator vessel, and apparent overall heat transfer coefficient of evaporator vessel.

Concerning the functions for physical properties, *etc.*, input of data can be made in two ways; either by giving values from a single curve or a set of corresponding curves, or by formulating the desired explicit expression with the aid of a so-called "external function". Using the first method, the program performs a curve-fitting procedure yielding the proper corresponding polynomials.

The demand for great flexibility has been fulfilled also by permitting seven basically different types of calculation cases. The actual type of calculation case is determined by INDUNS from an analysis of the input data. Hence the user is not obliged to be familiar with the different cases. Two of the cases are evaluation cases and the others are different types of design calculations.

In order to diminish the risk of feeding INDUNS with false or incomplete data, a thorough test of the input data is performed. If a mistake is discovered, a self-explanatory diagnostic message is printed out. There are about 50 different diagnostic messages, and the connection matrix, the input data matrix, as well as the functions for physical data are tested.

The demand for assured convergence has been fulfilled by using a special subroutine, ADJUST¹² (Jernqvist, 1975). This subroutine was developed at The Department of Chemical Engineering, Lund Institute of Technology, and is used mainly for the control of the estimations made in the iterative loop, but also for the control of internal, oscillating variables. One of the features of ADJUST is the calculation of an optimal relaxation factor.

INDUNS is written in FORTRAN V and was developed on the UNIVAC 1108 at the Lund Computing Center. However, no non-standard FORTRAN facilities, such as special library routines, have been used. Thus INDUNS may very well be used on other types of computer systems. The program comprises about 5400 punch cards divided into 51 subprograms, and it requires about 35000 decimal words of core memory. Typical computer running times are 5 to 50 seconds.

A comprehensive description of INDUNS is given in an internal report¹¹ (Bolmstedt, 1972). Besides, a separate user's manual¹³ (Bolmstedt, 1974a), is available.

Application of the program

INDUNS has been thoroughly tested using data from design as well as evaluation calculations found in the literature. Furthermore, the program has been used by students at the Department of Chemical Engineering, Lund Institute of Technology, for solution of problems concerning the design of multiple effect evaporation plants. These runs have shown that INDUNS is easily handled even by the inexperienced user, and that the diagnostic system of the program is very helpful and time-saving.

As for calculations of industrial plants, INDUNS has been used for both design and evaluation calculations in the sugar as well as in the kraft pulp industry. The complicated vapour distribution and heat recovery systems, which are used in the sugar industry in connection with the evaporation plant, can be easily accounted for with the aid of the flexible unit cell of INDUNS.

Recently, a great number of runs were carried out in the design of the rebuilding of two Swedish black liquor evaporation plants. The purpose of the first series of calculations was to find the vapour and liquor flow schemes giving the highest capacity expressed as thin liquor rate. In these calculations, the plant economy was not the most important factor. However, in the second series of calculations, the purpose was to determine the vapour and liquor flow schemes giving the best economy, *i.e.* the smallest live steam consumption for the desired rate of water evaporated, as well as the smallest rebuilding costs.

In both series of design calculations a special subfunction for the estimation of the overall heat transfer coefficients was used. The subfunction, called HTOT¹⁴ (Gudmundson, 1973), was developed at the Department of Chemical Engineering at Chalmers University of Technology and has been incorporated in INDUNS in a collaborative research project. This project, and the results from the first series of design calculations, are presented in Part I.

The second series of design calculations was carried out in cooperation with Svenska Cellulosa Aktiebolaget (SCA) for the black liquor evaporation plant at Munksund. Furthermore, two series of design calculations have been carried out in cooperation with the Swedish Steam Users' Association. These calculations were concerned with the design of new plants for black liquor evaporation. The ideas presented in Part I were used in the design work of both projects.

DYNAMIC SIMULATION

With respect to multiple effect evaporation plants, the main purpose of a steady-state simulation is to determine the proper heating areas of evaporators and heat exchangers, as well as the proper liquid and vapour schemes. However, many other important design parameters cannot be determined from steady-state simulations. Such parameters are liquid holdups of evaporators and storage tanks, control schemes and controller settings, *etc.* These parameters may however be determined from dynamic simulations, and it is therefore clear that a combination of steady-state and dynamic simulations would facilitate a proper design.

Although a number of investigations concerned with the dynamic behaviour of evaporators has been presented in the literature in the years 1960 to 1973, no program for simulation of the dynamic behaviour of general multiple effect evaporation plants has yet been reported. Instead, almost all of the papers published so far are concerned with the derivation and verification of either empirical or analytical models of single and double effect evaporators. Empirical transfer-function models were developed by *e.g.* Johnson¹⁵ (1960), Kropholler and Spikins¹⁶ (1965), and Park *et al.*¹⁷ (1972). The first more comprehensive model analysis was presented by Andersen *et al.*¹⁸ (1961). A single effect evaporator was described by five first-order ordinary differential equations. After reduction and linearization, the model was used for simulation and control purposes, with the aid of an analog computer. Andre and Ritter¹⁹ (1968) and Ritter and Andre²⁰ (1970) performed theoretical and experimental studies on a double effect evaporator. By neglecting vapour and heat transfer dynamics, a fifth-order model was obtained. In the first paper, the open-loop response was studied. The model and the actual plant showed excellent agreement in the liquid flow and concentration dynamics. In the second paper, the original non-linear model was compared with the linearized model. Discrepancies were noticed in amplitude, phase, and final steady-state value for the closed-loop system studied. Newell and Fisher²¹ (1972) discussed derivation and development of general evaporator models, and they suggested a modular approach. Measurements from a double effect evaporator (essentially the same equipment as used by Andre and Ritter) were compared with results obtained using a number of both linear and non-linear models of different orders. In conclusion, they found that the liquid flow and concentration dynamics were well described by a fifth-order non-linear model, and that linearized models gave quite unsatisfactory results in some cases.

The computer program DYNEFF

The main objective of the present work was to develop a computer program for simulation of the open-loop responses of general multiple effect evaporation plants. The program, called DYNEFF, uses INDUNS for the calculation of all necessary steady-state initial data. These data, as well as the flow-sheet data, are transferred to DYNEFF *via* a data storage file.

DYNEFF consists of a number of "dynamic blocks" comprising the necessary differential and algebraic equations for the components of the unit cell, and an "administrative part" governing the input/output procedures, the solution procedures, *etc.* This modular approach, and the sequential solution technique applied, provide handling of systems of apparently high order. The development of DYNEFF is presented in Part II.

The analysis of the analytical models presented so far showed that all the models are basically of the same nature. For instance, lumped-parameter first-order differential equations are the only type used, for long-tube as well as short-tube evaporators. Since the present work is concerned with the modeling of general evaporation plants, it was considered appropriate to use the ideas and results already presented, as a basis for the derivation of a proper evaporator model. The results obtained by Andre and Ritter¹⁹ (1968), Ritter and Andre²⁰ (1970), and Newell and Fisher²¹ (1972) indicated that the following assumptions were suitable for the derivation of a dynamic model of the evaporator vessel:

- vapour dynamics negligible (a)
- heat transfer surface heat capacity negligible (b)
- perfect mixing of liquid (c)
- vapour and liquid always in phase equilibrium (d)

Andre and Ritter¹⁹ (1968) proved the validity of assumptions (a) and (b) by calculating the time-constants for the steam chest, the vapour space, and the heat transfer surface dynamics. The calculated time-constants were found very small compared to those of the liquid holdup. Hence it seemed appropriate for the present work to extend the validity of assumptions (a) and (b) to a "general" evaporator model. As for assumption (c), its validity is highly dependent on the internal circulation rate and the liquid viscosity. The assumption of perfect mixing has however proved to be valid for short-tube as well as long-tube evaporators. To some extent this justifies the use of the perfect-mixing assumption for a "general"

model. Besides, if imperfect mixing is taken into account, the increase of model complexity and of necessary computer running time will be appreciable. Finally, assumption (d) is valid as long as pressure changes are small enough. It is hardly possible to take large and rapid pressure changes into account, since the effects of such changes are very complex.

Based on the above assumptions, a fourth-order model was developed for the evaporator vessel, shown in figure 2. Differential equations were derived for the following variables:

total mass	(M_L)
liquid enthalpy	(h_L)
concentration	(x_L)
metal wall temperature	(T_W)

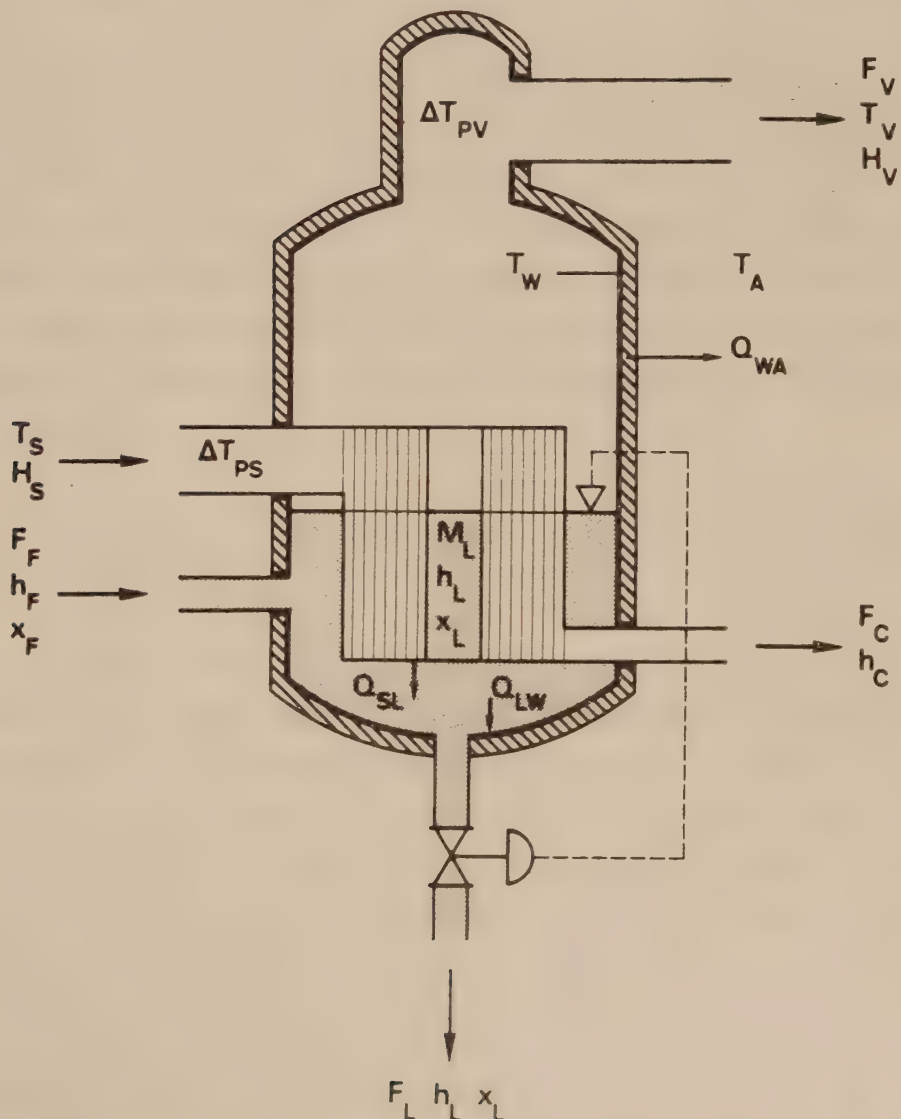


Figure 2. The evaporator vessel model

With this approach, an eighth-order model is obtained for a double effect evaporator, compared with the fifth-order models previously discussed. The higher order for the model presented here is due to the metal wall energy balances for both effects and the liquid energy balance for the second effect. The latter equation is omitted in the fifth-order models, based on the assumption of constant boiling temperature in the second effect.

The development of the mathematical models for the remaining components of the unit cell was to some extent based on the previous discussion. For instance, the assumption of very fast vapour dynamics makes a dynamic model for the vapour division vessel unnecessary. Hence the model for this vessel is based on steady-state equations. Moreover, the vapour dynamics of the flash tank and the heat exchanger is also neglected, and the necessary equations are based on steady-state relationships. All the models are used in their non-linear form.

As seen from figure 2, a liquid level controller is incorporated in the evaporator vessel model. Liquid level controllers are also included in the liquid mixing/division vessel model and in the condensate level controller model. For the heat exchanger, the liquid volume holdup is assumed to be constant, since this probably yields the best description of the liquid flow dynamics of most heat exchangers. The liquid mass holdup for the flash tank is considered constant, since no appropriate general vapour flow rate equation is available.

Two other controllers that should be considered in the dynamic modeling are the steam pressure and the condenser pressure controllers. Since the steam pressure controller in most cases reacts directly to the steam pressure, and hence is very fast, it is omitted in the present work. For the condenser, however, liquid dynamics is normally involved, and consequently the time-constants for the condenser dynamics may be of the same magnitude as for any other liquid dynamics in the system. It therefore seemed appropriate to take the condenser dynamics into account. For reasons of computational and modeling simplicity, however, the condenser is not completely modeled. Instead, the controller equation for the condenser pressure is designed to describe both the condenser dynamics and the controller function, and is incorporated in the evaporator vessel model. All controller equations are designed on the basis of ordinary PI-controllers. Arbitrary values of the proportional constants and of the integration times may be defined in the

input data to DYNEFF, and hence the controller equations can simulate any combination of proportional and integrational control. The controller constants defined in the input data are specific for each controller.

The integration of the differential equations is carried out with the aid of a weighted residual method, namely the orthogonal collocation method. In an earlier investigation²² (Bolmstedt, 1974b), this method was thoroughly tested on a simple chemical engineering system. The main objective of the investigation was to examine the applicability of the method to coupled first-order ordinary non-linear differential equations, forming a rather stiff system. The orthogonal collocation method proved to be very powerful, and even when very large time steps were used, numerical instability did not occur. Furthermore, almost regardless of the number of collocation points (*i.e.* the order of the approximation polynomial) and the size of the time step, the calculated results were always within "engineering accuracy". Besides, the necessary computer running times were moderate, and hence the method was considered well suited for use in the present work. The theories of weighted residual methods in general, and the orthogonal collocation method in particular, are discussed by Villadsen^{23,24} (1973a,b). The FORTRAN subroutines necessary for the calculation of collocation points, differential operators, *etc.*, are taken from Michelsen²⁵ (1973), and developed for use in the present work. The orthogonal collocation method yields a system of non-linear algebraic equations. The equation system must be solved iteratively, and applicable techniques are, in principle, for instance Newton's method and successive approximation. In the present work Newton's method is almost impossible to use. This is due mostly to the fact that the algebraic functional relationships for physical properties are not analytically known. Hence it may be very difficult to calculate the partial derivatives required for Newton's method. Instead, Gaussian elimination coupled with subroutine ADJUST for correction of the solution vector is employed.

DYNEFF is written in FORTRAN V and was developed on the UNIVAC 1108 at the Lund Computing Center. The program comprises about 3700 punch cards divided into 48 subprograms, and it requires about 40000 decimal words of core memory. A comprehensive description of the program is given in an internal report²⁶ (Bolmstedt, 1974c). The report includes a user's manual.

Suggested application of the program

The main objective of the project was to develop a computer program for simulation of open-loop responses of general multiple effect evaporation plants. The use of the program will increase the possibilities of achieving better knowledge and understanding of the dynamic behaviour of evaporation plants in general. Moreover, the effects of changed controller settings, liquid holdups, piping, *etc.*, may be studied using the program. Hence it should be possible to use the program in equipment design and in the determination of controller settings of the internal controllers. It should also be possible to use the program for identification purposes, and thus facilitate for instance the derivation of low-order transfer functions describing the dynamic behaviour of a complex, high-order system. A low-order transfer-function model is more applicable to computer control.

In Part II a numerical example concerning the open-loop response of a quadruple effect plant is given. The plant flow sheet is shown in figure 3. Besides the evaporator vessels, there are two heat exchangers, two storage tanks, and two flash tanks included in the plant. A 10 per cent upset

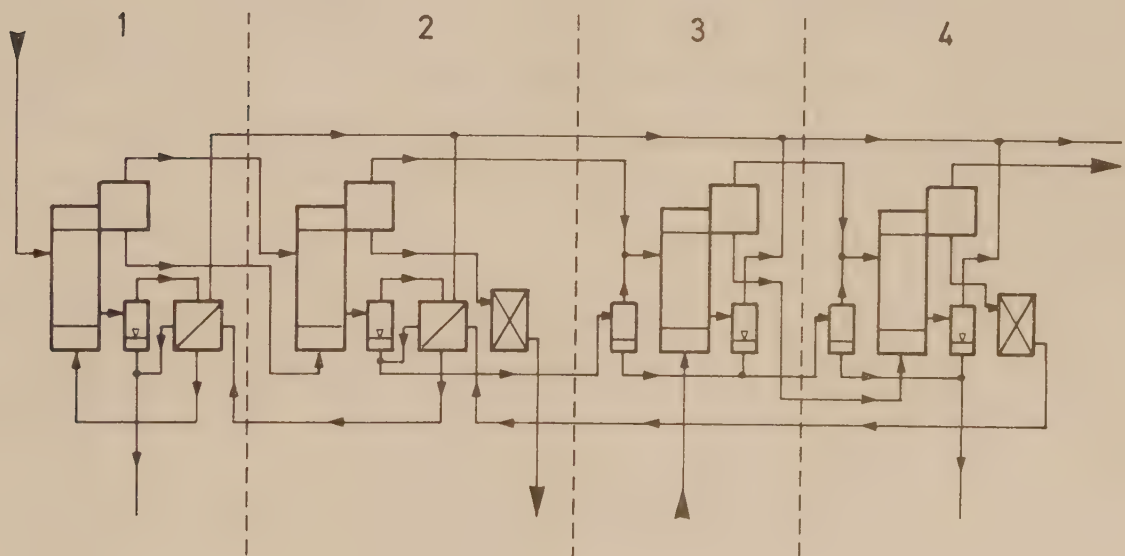


Figure 3. Flow sheet of quadruple effect plant

in the feed flow rate was used as input signal. The responses studied are concerned with the liquid flow, the concentration, and the temperature dynamics of the plant. As an example of the results obtained from the simulation run, the concentration responses for the evaporator vessels and the

storage tanks are shown in figure 4. The numbers refer to the respective unit cells.

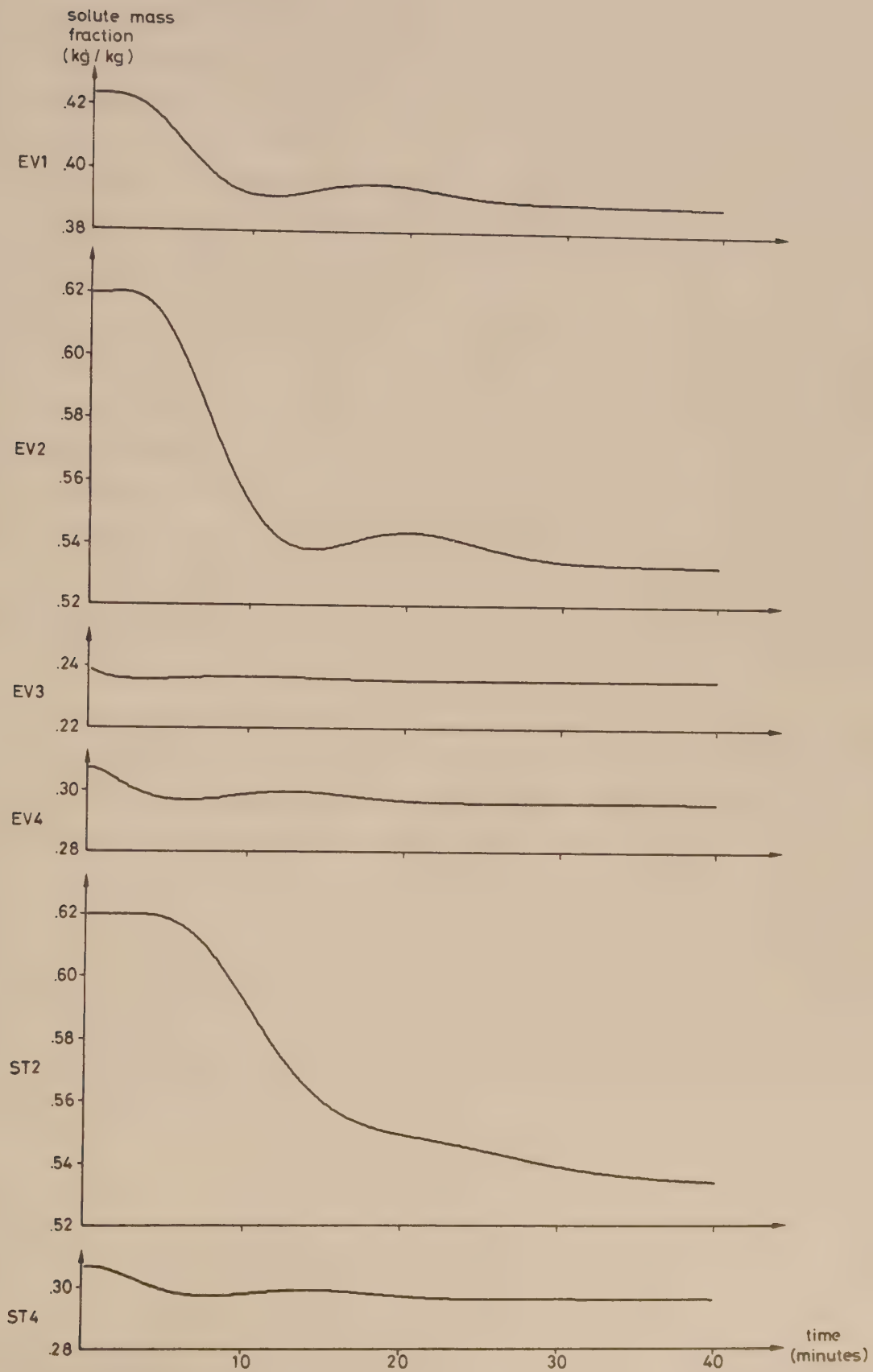


Figure 4. Responses of concentration for evaporator vessels (EV) and storage tanks (ST) to a 10 per cent upset in feed flow rate

FUTURE DEVELOPMENT

In Part I the results from a series of design calculations of black liquor evaporation plants are presented. It is shown that the use of overall heat transfer coefficients estimated from plants in normal operation is very uncertain, when the vapour and liquor schemes are radically changed. With the use of a subfunction for accurate estimation of the heat transfer coefficients, in the present case the subfunction HTOT, plants diverging from normal layout can be accurately design calculated. Hence the possibilities of obtaining an optimal design are greatly increased. The subfunction HTOT is however only applicable to black liquor Kestner evaporators, and thus INDUNS would gain in flexibility if a "general" subfunction for the calculation of overall heat transfer coefficients were incorporated in the program. In fact, this problem is being dealt with in a research project now underway at the Department of Chemical Engineering, Lund Institute of Technology. The project is concerned with energy optimization in chemical engineering, and includes investigation of vapour recompression in multiple effect evaporation, with the aid of INDUNS and a function of the type mentioned. With this subfunction incorporated in INDUNS, it should be possible to accurately design calculate any multiple effect evaporation plant.

The computer program DYNEFF, presented in Part II, is designed primarily for the simulation of open-loop responses of general multiple effect evaporation plants. However, due to the strictly modular construction of the program, further development may be easily carried out. For instance, DYNEFF may be modified to simulate closed-loop responses as well, and thereby facilitate the design of suitable controller algorithms, for example for product concentration control. Furthermore, the "dynamic blocks" may be partly or completely changed, in case other mathematical models are desired. For more specific applications, the program can be much simplified with respect to its administrative parts. Hence the necessary computer running times will be decreased.

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Ulf Bolmstedt

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